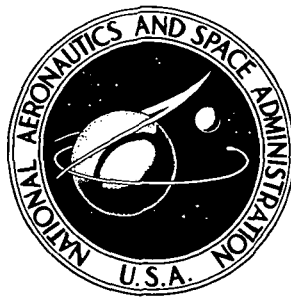


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**FIGURE-OF-MERIT CALCULATION METHODS  
FOR ORGANIC HEAT-PIPE FLUIDS**

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# FIGURE-OF-MERIT CALCULATION METHODS FOR ORGANIC HEAT-PIPE FLUIDS

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## SUMMARY

With only chemical formulas and operating temperatures specified, selected correlating equations and tables of chemistry-effect functions allow estimates of figures of merit for organic heat-pipe fluids.

## INTRODUCTION: SELECTING ORGANIC HEAT-PIPE FLUIDS

Some organic chemicals perform adequately as heat-pipe fluids and offer special application advantages (refs. 1 to 3). The heat-pipe potentialities of such compounds depend on their properties as indicated by the simple figures of merit described in reference 4:

"zero-g figure of merit" or "liquid transport factor":

$$L = \frac{\sigma_l \rho_l \lambda_l}{\mu_l} \quad (1)$$

"g-field figure of merit":

$$G = \frac{\sigma_l}{\rho_l} \quad (2)$$

"nucleation tolerance factor":

$$N = \frac{k_l \sigma_l}{\lambda_l \rho_v} \quad (3)$$

where  $\sigma_l$  is surface tension,  $\rho_l$  is density,  $\lambda_l$  is latent heat of vaporization,  $\mu_l$  is viscosity,  $k_l$  is thermal conductivity - all of the liquid; and  $\rho_v$  is saturated-vapor density.

Equations (1) to (3) are convenient for screening heat-pipe fluids. However, tabulations of the properties necessary to compute these figures of merit over wide temperature variations are often unavailable for less common organic compounds. Fortunately references 5 and 6 provide correlations collected from numerous sources to predict physical characteristics of various chemicals as functions of molecular formulas and operating temperatures only. So this minimal information allows estimations and comparisons of heat-pipe figures of merit for organic fluids. The present report comprises selections of appropriate equations, conversions, and chemistry-effect functions to enable such screening.

## CALCULATION METHODS: PHYSICAL PROPERTIES AND FIGURES OF MERIT

Unless otherwise indicated input variables and results of the following equations bear international units (SI, mksa). Using this system required numerous conversions in the physical-property correlations, which come from long-established chemical-engineering references (refs. 5 and 6). And because these expressions relate to chemistry and thermodynamics, the concept of the mol naturally arises: the cgs gram-mol, the British pound-mol, but the mksa gram-mol (ref. 7) not the mksa kilogram-mol. So the molecular weight  $M$  appears here as grams per gram-mol. This detail is, of course, very important in preventing thousandfold errors during kilogram transformations of the many mol-based characteristics.

Except  $M$  and the gas constant  $R$  ( $8.314 \text{ (J)(K}^{-1}\text{)(mol}^{-1}\text{)}$ ), though, the dimensions of the physical properties in this report involve only the usual mksa units ( $C_p$ ,  $(\text{J})(\text{kg}^{-1})(\text{K}^{-1})$ ;  $k$ ,  $(\text{J})(\text{m}^{-1})(\text{sec}^{-1})(\text{K}^{-1})$ ;  $P$ ,  $(\text{N})(\text{m}^{-2})$ ;  $T$ ,  $\text{K}$ ;  $\lambda$ ,  $(\text{J})(\text{kg}^{-1})$ ;  $\mu$ ,  $(\text{N})(\text{sec})(\text{m}^{-2})$ ;  $\rho$ ,  $(\text{kg})(\text{m}^{-3})$ ; and  $\sigma$ ,  $(\text{N})(\text{m}^{-1})$ ). The appendix defines the symbols, and reference 5 gives unconverted versions of equations (4) to (23).

## INPUT VARIABLES

Computing figures of merit for an organic heat-pipe fluid begins with specification of the chemical formula (CF) and the operating temperature  $T_l$  of the liquid. Usually the normal boiling point  $T_b$  is also available through the literature or simple testing. And because correlations leading to  $k_l$ ,  $\lambda_l$ ,  $\mu_l$ ,  $\sigma_l$ ,  $\rho_l$ , and  $\rho_v$  depend strongly on  $T_b$  a well-determined value of this variable is desirable. But if such a  $T_b$  is lacking, the first equation of the next section yields a reasonable estimate.

## NORMAL-BOILING AND CRITICAL POINTS

Equations for normal-boiling and critical points are given in this section.

Normal boiling temperature:

$$T_b = \frac{637 [R_D]^{1.47} + B}{[P]} \quad (4)$$

The parachor  $[P]$  and molar refraction  $[R_D]$  are sums of CF effects taken directly from table 3-285 of reference 5 (or table 3-287 for  $[P]$ ). And  $B$  is a chemistry-dependent constant from table 3-286.

Critical-point temperature and pressure:

$$T_c = \frac{T_b}{\frac{\Sigma \Delta_T}{100}} \quad (5)$$

$$P_c = \frac{1.013 \times 10^9 \text{ M}}{(\Sigma \Delta_P)^2} \quad (6)$$

Here again  $\Sigma \Delta_T$  and  $\Sigma \Delta_P$  result from summations of CF contributions listed in tables 3-288 and 3-289 of reference 5.

Normal-boiling-point latent heat of vaporization:

$$\lambda_b = \frac{RT_c T_b \ln \frac{P_c}{1.013 \times 10^5}}{(T_c - T_b)M \times 10^{-3}} \quad (7)$$

Critical-point compressibility factor and density:

$$Z_c = \frac{1}{3.43 + 0.0067 \left( \frac{\lambda_b M}{4.184 \times 10^6} \right)^2} \quad (8)$$

$$\rho_c = \frac{P_c}{Z_c R T_c} M \times 10^{-3} \quad (9)$$

Normal-boiling-point liquid density:

$$\rho_{l,b} = \rho_c \left( 1.981 + 0.422 \log \frac{P_c}{1.013 \times 10^5} \right) \quad (10)$$

Having these normal-boiling and critical characteristics enables the following evaluations of physical properties necessary to compute the heat-pipe figures of merit.

#### SATURATED-FLUID PROPERTIES AT LIQUID OPERATING TEMPERATURE

Saturated-fluid properties at liquid operating temperatures are given in this section.

Saturated-vapor pressure and density:

$$P_v = P_c \left( \frac{T_l}{T_c} \right)^{\alpha'} \times 10^{(0.137 - 0.0364\alpha')B'} \quad (11)$$

where

$$B' = 36 \frac{T_c}{T_l} - 35 - \left( \frac{T_l}{T_c} \right)^6 + 42 \ln \frac{T_l}{T_c} \quad (12)$$

and

$$\alpha' = 0.878 + 2.11 \frac{\log \frac{P_c}{1.013 \times 10^5}}{\frac{T_c}{T_b} - 1} \quad (13)$$

The compressibility factor  $Z_v$  is now required to obtain the saturated-vapor density  $\rho_v$  from the corresponding pressure  $P_v$  and temperature  $T_l$ . Table I worked up from data presented in reference 6 allows interpolations of  $Z_v$  as a function of  $Z_c$ ,  $T_{l,r} = T_l/T_c$ , and  $P_{v,r} = P_v/P_c$ . Then

$$\rho_v = \frac{P_v M \times 10^{-3}}{Z_v R T_l} \quad (14)$$

Liquid density:

$$\rho_l = (\rho_{l,b} - \rho_{v,b}) \left( \frac{T_c - T_l}{T_c - T_b} \right)^{1/3} + \rho_v \quad (15)$$

The saturated-vapor density at the normal boiling point  $\rho_{v,b}$  results from equation (14) and the preceding paragraph used with  $T_b$  and  $P_{v,b} = 101\,325$  newtons per square meter.

Surface tension:

$$\sigma_l = \left[ \frac{[P](\rho_l - \rho_v)}{M} \right]^4 \times 10^{-15} \quad (16)$$

For this equation a summation of CF effects taken from table 3-294 of reference 5 produces the parachor  $[P]$ .

Latent heat of vaporization:

$$\lambda_l = \frac{RT_c T_b}{M \times 10^{-3}} \left( \ln \frac{P_c}{1.013 \times 10^5} \right) \frac{(T_c - T_l)^{0.38}}{(T_c - T_b)^{1.38}} \quad (17)$$

Constant-pressure specific heat and thermal conductivity:

$$C_{p,l} = C_{p,l,20} \left( \frac{1 - \frac{140.7}{T_c}}{1 - 0.48 \frac{T_l}{T_c}} \right)^{2.8} \quad (18)$$

Summing CF contributions from table 3-291 of reference 5 and multiplying by 4184/M give the liquid specific heat at 20° C to be used in equation (18). With the resulting  $C_{p,l}$

$$k_l = \frac{4.27 C_{p,l} \rho_l^{4/3}}{\alpha M^{1/3}} \times 10^{-8} \quad (19)$$

where

$$\alpha = \alpha_{30} - (\alpha_{30} - 1) \left[ \frac{T_c - T_l}{T_c - 303.15 \left( \text{or } \frac{T_c}{2} \right)} \right] = \frac{\lambda_b M}{T_b \times 8.8 \times 10^4} \left[ \frac{T_l - 303.15 \left( \text{or } \frac{T_c}{2} \right)}{T_c - 303.15 \left( \text{or } \frac{T_c}{2} \right)} \right] + \frac{T_c - T_l}{T_c - 303.15 \left( \text{or } \frac{T_c}{2} \right)} \quad (20)$$

unless this value is less than unity; then  $\alpha = 1.0$  is used. And



$$\alpha_{30} = \frac{\lambda_b M}{T_b \times 8.8 \times 10^4} \quad (21)$$

according to reference 5, which indicates that this constant applies "at 30° C for most liquids or at  $T_c/2$  for low boilers such as methane,  $N_2$ , and ethylene . . . . Calculated values of  $\alpha < 1$  should be taken as unity, and at temperatures other than 30° C (or  $T_c/2$ ),  $\alpha$  may be assumed to vary linearly between values given by the Eq. [(21)] at 30° C and 1.0 at  $T_c$ ."

Liquid viscosity:

$$\mu_l = 1.167 \rho_l^{1/2} \times 10^{B'' \left( \frac{T_c}{T_l} - 1 \right) - \frac{11}{2}} \quad (22)$$

where  $B''$  is another sum of CF effects from table 3-297 of reference 5.

#### FIGURES OF MERIT

Substituting fluid-property values from the equations of the preceding section into equations (1) to (3) yields figures of merit for organic heat-pipe fluids:

$$L = \frac{\sigma_l \rho_l \lambda_l}{\mu_l} = \frac{(16)(15)(17)}{(22)} \quad (1')$$

$$G = \frac{\sigma_l}{\rho_l} = \frac{(16)}{(15)} \quad (2')$$

$$N = \frac{k_l \sigma_l}{\lambda_l \rho_l} = \frac{(19)(16)}{(17)(14)} \quad (3')$$

#### DISCUSSION: USE OF CALCULATED FLUID PROPERTIES AND FIGURES OF MERIT

The selected correlations for physical properties involve generally modest average errors, which references 5 and 6 discuss. But the question of accuracy is a moot one

since these expressions are of value only in the absence of the necessary compilations of experimental data.

When such collections of physical properties are unavailable, an initial screening with only  $L$  (eq. (1')) and  $G$  (eq. (2')) estimates seems appropriate for conventional heat pipes. Then  $N$  (eq. (3')) comparisons for the more promising fluids would further reduce the field. This is a desirable approach because  $L$  is the most widely used figure of merit, because  $G$  bolsters the meaning of  $L$  and depends only on results necessary to compute  $L$ , and because  $k_l$  and  $\rho_v$  required for  $N$  involve time-consuming calculations.

Neglecting  $\rho_v$  at the outset simplifies the calculations of  $\rho_l$  (eq. (15)) and  $\sigma_l$  (eq. (16)) and limits the initial screening to heat pipes where  $\rho_v \ll \rho_l$ . But this condition generally applies because the liquid pumping potential  $\sigma_l$  (eq. (16)) decreases very rapidly as  $\rho \rightarrow \rho_v$ .

Incidentally, the ratio form for the correlation of density differences

$$\frac{\rho_l - \rho_v}{\rho_{l,b} - \rho_{v,b}} = \left( \frac{T_c - T_l}{T_c - T_b} \right)^{1/3} \quad (15')$$

is quite similar to that for latent heats of vaporization:

$$\frac{\lambda_l}{\lambda_b} = \left( \frac{T_c - T_l}{T_c - T_b} \right)^{0.38} \quad (23)$$

This comparison indicates clearly that the heat pipe becomes less effective as the density of the vapor increases toward that of the liquid - because simultaneously the heat of vaporization approaches zero. So heat pipes, which essentially transport the enthalpy of condensation, should operate with  $\rho_v \ll \rho_l$ . Consequently, neglecting  $\rho_v$  effects in the suggested initial screening is a justifiable economy.

These simplifications used with the selected physical-property correlations and the figure-of-merit expressions allow meaningful first-round evaluations of unusual organic heat-pipe fluids.

Lewis Research Center,

National Aeronautics and Space Administration,

Cleveland, Ohio, September 18, 1973,

503-25.

## APPENDIX - SYMBOLS

B	CF-dependent constant
B'	function of reduced temperature $T_l/T_c$ in vapor-pressure equation
B''	sum of CF effects in liquid-viscosity equation
$C_{p,l}$	constant-pressure specific heat for liquid
$C_{p,l,20}$	constant-pressure specific heat for 20° C liquid
G	G-field figure of merit
$k_l$	thermal conductivity of liquid
L	liquid transport factor (zero-g figure of merit)
M	molecular weight
N	nucleation tolerance factor
[P]	parachor, sum of CF effects in normal-boiling-temperature and surface-tension equations
$P_c$	pressure at critical point
$P_v$	saturated-vapor pressure at $T_l$
$P_{v,b}$	saturated-vapor pressure at normal boiling point
R	gas constant
$[R_D]$	molar retraction, sum of CF effects in normal-boiling-temperature equation
$T_b$	normal-boiling temperature
$T_c$	critical-point temperature
$T_l$	liquid operating temperature
$Z_c$	critical-point compressibility factor
$Z_v$	compressibility factor of saturated vapor at $T_l$
$\alpha$	functional factor in thermal-conductivity equation
$\alpha_{30}$	functional factor at 30° C (or $T_c/2$ ) in thermal-conductivity equation
$\alpha'$	functional factor in exponents of vapor-pressure equation
$\lambda_b$	latent heat of vaporization at normal boiling point
$\lambda_l$	latent heat of vaporization at $T_l$
$\mu_l$	liquid viscosity at $T_l$
$\rho_c$	critical-point density

$\rho_l$	liquid density at $T_l$
$\rho_{l,b}$	liquid density at normal boiling point
$\rho_v$	saturated-vapor density at $T_l$
$\rho_{v,b}$	saturated-vapor density at normal boiling point
$\Sigma\Delta_p$	sum of CF effects in critical-point-pressure equation
$\Sigma\Delta_T$	sum of CF effects in critical-point-temperature equation
$\sigma_l$	liquid surface tension at $T_l$

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TABLE I. - COMPRESSIBILITY FACTORS FOR SATURATED VAPORS

Reduced saturated-vapor pressure at $T_l$ , $P_{v,r} = P_v/P_c$	Critical-point compressibility factor, $Z_c$							
	0.23		0.25		0.27		0.29	
	Reduced liquid operating temperature, $T_{l,r} = T_l/T_c$	Compressibility factor of saturated vapor at $T_l$ , $Z_v$	Reduced liquid operating temperature, $T_{l,r} = T_l/T_c$	Compressibility factor of saturated vapor at $T_l$ , $Z_v$	Reduced liquid operating temperature, $T_{l,r} = T_l/T_c$	Compressibility factor of saturated vapor at $T_l$ , $Z_v$	Reduced liquid operating temperature, $T_{l,r} = T_l/T_c$	Compressibility factor of saturated vapor at $T_l$ , $Z_v$
0.1	0.769	0.872	0.759	0.893	0.738	0.901	0.712	0.902
.2	.825	.810	.816	.830	.802	.837	.777	.839
.3	.863	.752	.856	.872	.845	.781	.827	.783
.4	.891	.700	.884	.727	.876	.738	.862	.742
.6	.937	.593	.932	.623	.927	.633	.919	.644
.8	.971	.480	.970	.505	.968	.521	.963	.533
.9	.986	.405	.986	.426	.984	.443	.982	.461
1.0	1.000	.230	1.000	.250	1.000	.270	1.000	.290



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